Models and Simulations of UO_2 Fuel Materials Properties

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Nuclear fuels are subject to severe radiation environments and their thermal, chemical, and mechanical properties change significantly with time and irradiation level [1]. The major factors that influence the properties are temperature, stoichiometry, and microstructure (especially porosity and point defects). In particular, the accumulation of fission products in gas bubbles can decrease the heat transfer, leading to overheating of the fuel element and local melting (Fig. 1).

This work is focused on the irradiation effects on properties such as thermal conductivity, oxygen diffusivity, and thermal expansion. Our methods cover a large spectrum of time and space scales, from electronic structure to atomistic, to meso-scale, to continuum (Fig. 2).

The results include electronic structure calculations of phonon spectra (Fig. 3), models of point defect concentrations, stoichiometry and diffusivity (Fig. 4), simulations of gas bubble formation and evolution (Fig. 5), and coupled simulations of heat transport, diffusion, and thermal expansion [6]. Future work will be focused on advanced, multi-component fuels that contain transuranic elements and fission products.

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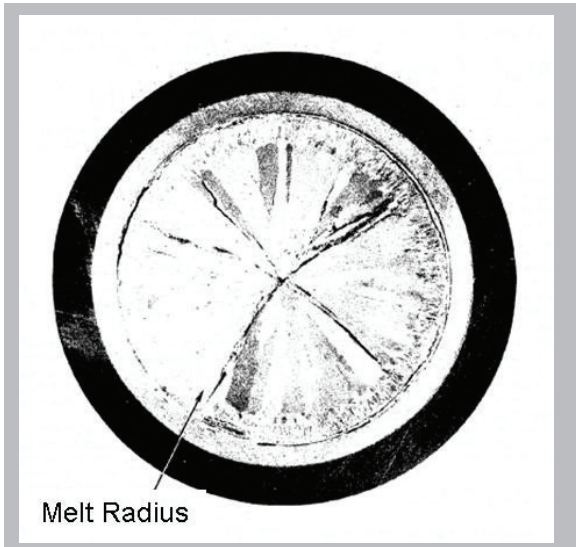

Fig. 1. Cross-section of UO_2 fuel rod operated at a linear power high enough to cause extensive melting [2].

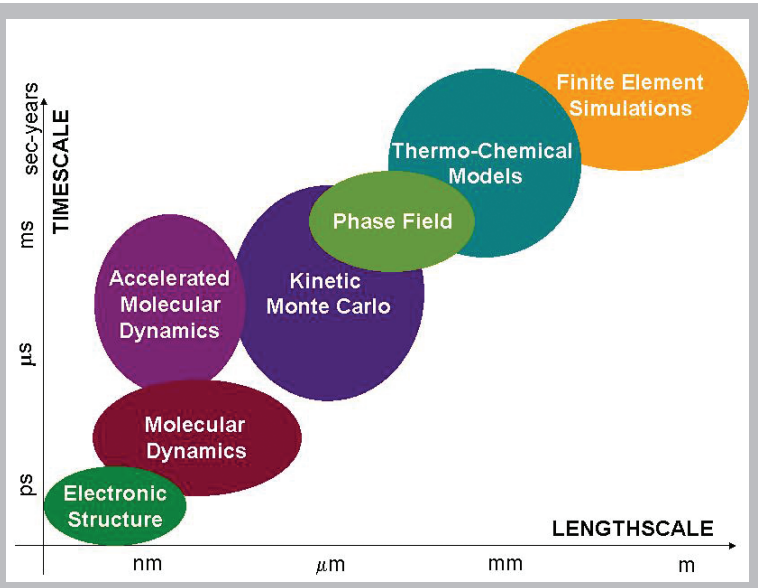

Fig. 2. In the multiscale approach the information is transferred via global properties such as density, thermal conductivity, and species mobility [3].

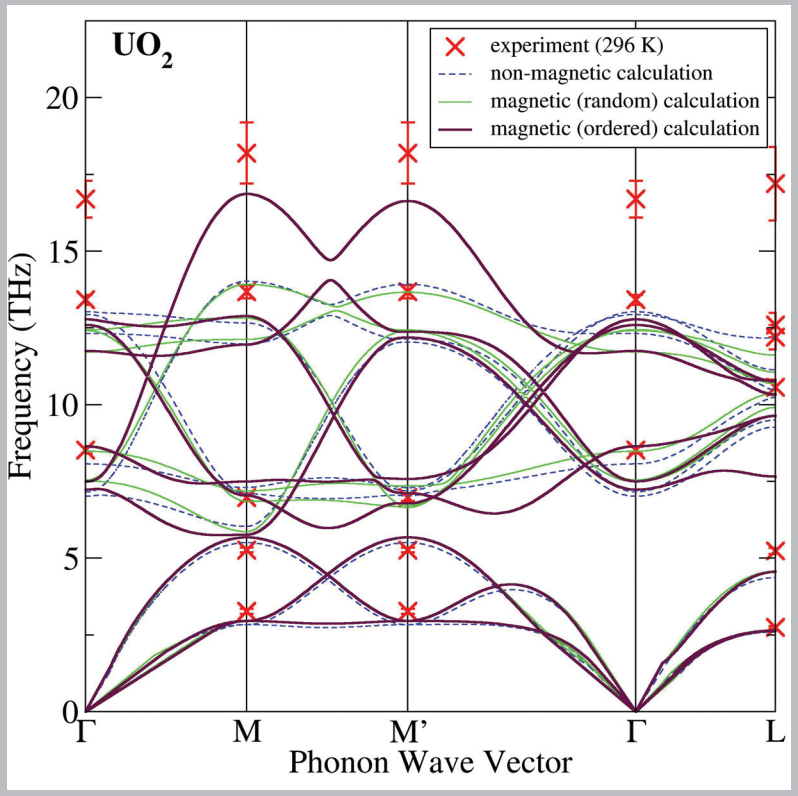

Fig. 3. Electronic structure calculations of phonon frequencies of UO_2. This is a complex material with properties determined by temperature, magnetic structure, strong spin-orbit coupling, and strongly correlated 5f electrons. The frequencies are used to determine thermal expansion and heat capacity of UO_2. Magnetic structure affects calculated energies and phonon frequencies significantly. These results indicate that magnetic moments must be included with specific structure [3].

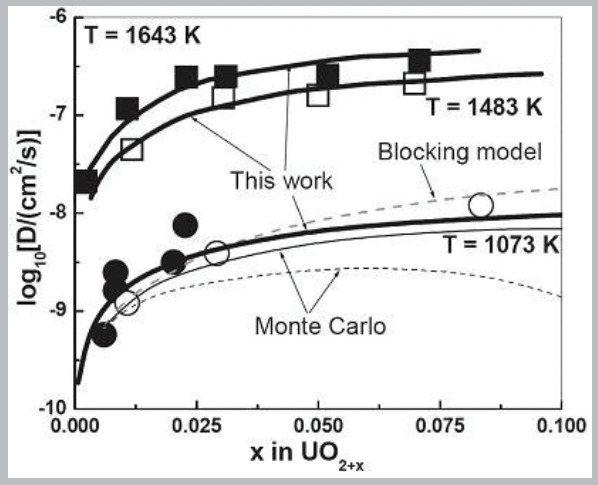

Fig. 4. Oxygen self-diffusivity as a function of non-stoichiometry (x in UO_{2+x}) and temperature. Solid line: our model [4]. Symbols: data from literature [4]. The model we have developed is valid for a large domain of temperature (300 K < T < 1800 K) and oxygen content (x < 0.1) [4].

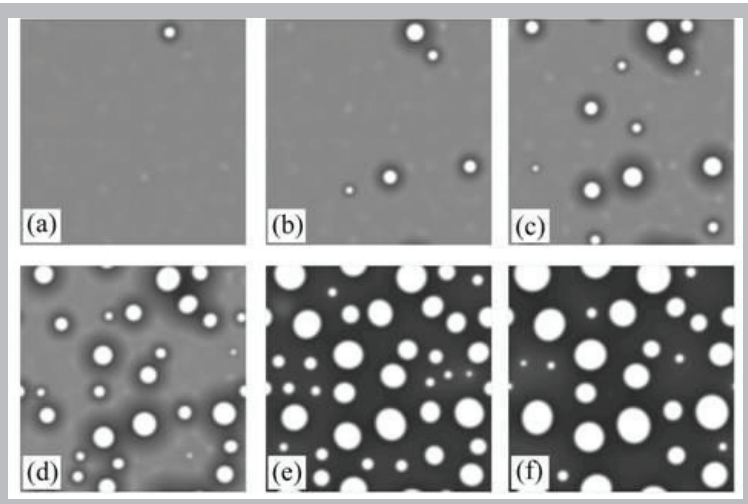

Fig. 5. Phase Field simulation of homogeneous nucleation and growth of gas bubbles. Characteristic time: (a) 10 s, (b) 50 s, (c) 100 s, (d) 150 s, (e) 250 s, and (f) 350 s. Next step is including microstructure features, especially grain boundaries [5].